W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 14, 2024 – 11:09 am GMT

PDB ID	:	6STZ
Title	:	Crystal structure of dimethylated RSLex - cucurbituril free form
Authors	:	Guagnini, F.; Engilberge, S.; Crowley, P.B.
Deposited on	:	2019-09-12
Resolution	:	1.14 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
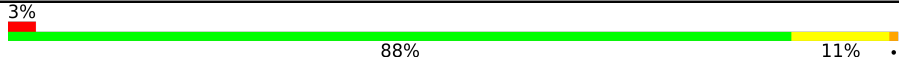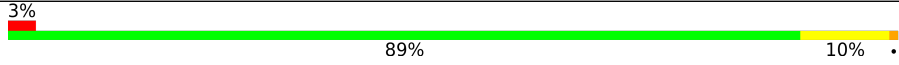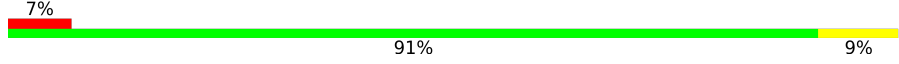*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.14 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
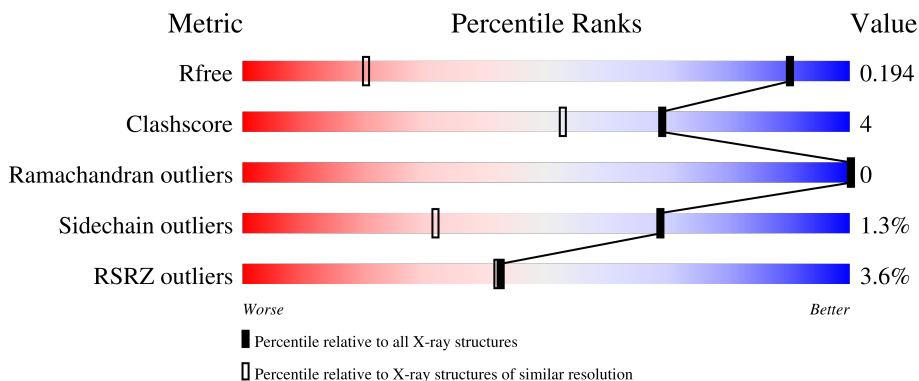
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1492 (1.18-1.10)
Clashscore	141614	1537 (1.18-1.10)
Ramachandran outliers	138981	1483 (1.18-1.10)
Sidechain outliers	138945	1480 (1.18-1.10)
RSRZ outliers	127900	1464 (1.18-1.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	89	
1	B	89	
1	C	89	
1	D	89	
1	E	89	

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Mol	Chain	Length	Quality of chain
1	F	89	92% 6% ·

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 5251 atoms, of which 144 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Fucose-binding lectin protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	89	Total	C	N	O	S	0	2	0
			707	450	119	136	2			
1	B	89	Total	C	N	O	S	0	0	0
			696	443	117	134	2			
1	C	89	Total	C	N	O	S	0	0	0
			695	443	117	133	2			
1	D	87	Total	C	N	O	S	0	0	0
			680	435	114	129	2			
1	E	88	Total	C	N	O	S	0	1	0
			694	443	116	133	2			
1	F	87	Total	C	N	O	S	0	0	0
			680	435	114	129	2			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	THR	SER	conflict	UNP A0A0S4WQH1
A	79	MLY	ASN	conflict	UNP A0A0S4WQH1
A	82	TYR	THR	engineered mutation	UNP A0A0S4WQH1
B	67	THR	SER	conflict	UNP A0A0S4WQH1
B	79	MLY	ASN	conflict	UNP A0A0S4WQH1
B	82	TYR	THR	engineered mutation	UNP A0A0S4WQH1
C	67	THR	SER	conflict	UNP A0A0S4WQH1
C	79	MLY	ASN	conflict	UNP A0A0S4WQH1
C	82	TYR	THR	engineered mutation	UNP A0A0S4WQH1
D	67	THR	SER	conflict	UNP A0A0S4WQH1
D	79	MLY	ASN	conflict	UNP A0A0S4WQH1
D	82	TYR	THR	engineered mutation	UNP A0A0S4WQH1
E	67	THR	SER	conflict	UNP A0A0S4WQH1
E	79	MLY	ASN	conflict	UNP A0A0S4WQH1
E	82	TYR	THR	engineered mutation	UNP A0A0S4WQH1
F	67	THR	SER	conflict	UNP A0A0S4WQH1
F	79	MLY	ASN	conflict	UNP A0A0S4WQH1

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Chain	Residue	Modelled	Actual	Comment	Reference
F	82	TYR	THR	engineered mutation	UNP A0A0S4WQH1

- Molecule 2 is beta-D-fructopyranose (three-letter code: BDF) (formula: $C_6H_{12}O_6$).

BDF

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 24	C 6	H 12	O 6	0	0
2	A	1	Total 24	C 6	H 12	O 6	0	0
2	B	1	Total 24	C 6	H 12	O 6	0	0
2	B	1	Total 24	C 6	H 12	O 6	0	0
2	C	1	Total 24	C 6	H 12	O 6	0	0
2	C	1	Total 24	C 6	H 12	O 6	0	0
2	D	1	Total 24	C 6	H 12	O 6	0	0
2	D	1	Total 24	C 6	H 12	O 6	0	0
2	E	1	Total 24	C 6	H 12	O 6	0	0
2	E	1	Total 24	C 6	H 12	O 6	0	0
2	F	1	Total 24	C 6	H 12	O 6	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	F	1	Total 24	C 6	H 12	O 6	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	131	Total 131	O 131	0	0
3	B	131	Total 131	O 131	0	0
3	C	136	Total 136	O 136	0	0
3	D	137	Total 137	O 137	0	0
3	E	144	Total 144	O 144	0	0
3	F	132	Total 132	O 132	0	0

WORLDWIDE
PDB
PROTEIN DATA BANK

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Fucose-binding lectin protein
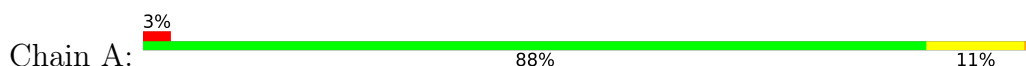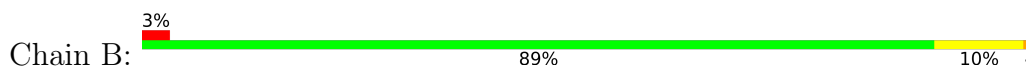
Chain A:

• Molecule 1: Fucose-binding lectin protein

Chain B:

• Molecule 1: Fucose-binding lectin protein

Chain C:

• Molecule 1: Fucose-binding lectin protein

Chain D:

• Molecule 1: Fucose-binding lectin protein

Chain E:

• Molecule 1: Fucose-binding lectin protein

Chain F:

92%   6%

S2 K25 K34 N47 K79 K83 S88 THR ASN
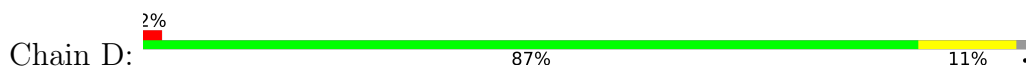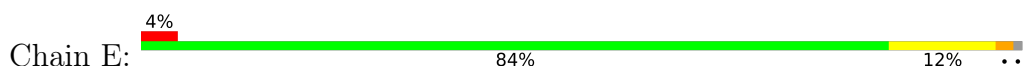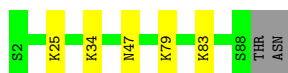
4 Data and refinement statistics ⓘ

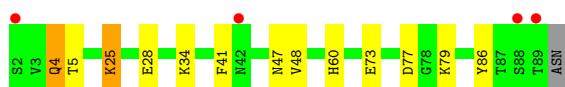| Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	43.95Å 43.95Å 207.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	69.09 – 1.14 69.09 – 1.14	Depositor EDS
% Data completeness (in resolution range)	99.8 (69.09-1.14) 99.8 (69.09-1.14)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.07 (at 1.14Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.173 , 0.198 0.175 , 0.194	Depositor DCC
R_{free} test set	8163 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	8.2	Xtriage
Anisotropy	0.516	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 50.6	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.47, < L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.016 for -h,-k,l 0.049 for h,-h-k,-l 0.035 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	5251	wwPDB-VP
Average B, all atoms (Å^2)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 59.12 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.8484e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BDF, MLY

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$>5	RMSZ	#$|Z|$>5
1	A	0.55	0/691	0.69	0/953
1	B	0.52	0/674	0.69	0/930
1	C	0.58	0/673	0.70	0/929
1	D	0.55	0/658	0.66	0/908
1	E	0.54	0/675	0.69	0/931
1	F	0.54	0/658	0.67	0/908
All	All	0.55	0/4029	0.68	0/5559

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	707	0	660	11	0
1	B	696	0	646	5	0
1	C	695	0	643	4	0
1	D	680	0	630	6	0
1	E	694	0	648	11	0
1	F	680	0	630	1	0
2	A	24	24	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	24	24	24	0	0
2	C	24	24	24	0	0
2	D	24	24	24	0	0
2	E	24	24	24	0	0
2	F	24	24	24	0	0
3	A	131	0	0	1	0
3	B	131	0	0	0	0
3	C	136	0	0	0	0
3	D	137	0	0	0	0
3	E	144	0	0	2	0
3	F	132	0	0	0	0
All	All	5107	144	4001	31	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 31 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:25:MLY:HG3	3:E:230:HOH:O	1.81	0.79
1:D:4:GLN:HE22	1:D:48:VAL:H	1.28	0.78
1:A:60:HIS:HD2	1:A:77:ASP:OD1	1.65	0.78
1:E:4[A]:GLN:HE22	1:E:48:VAL:H	1.32	0.78
1:E:60:HIS:HD2	1:E:77:ASP:OD1	1.74	0.70

There are no symmetry-related clashes.

5.3　Torsion angles ⓘ

5.3.1　Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	85/89 (96%)	85 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	83/89 (93%)	82 (99%)	1 (1%)	0	100	100
1	C	83/89 (93%)	81 (98%)	2 (2%)	0	100	100
1	D	81/89 (91%)	81 (100%)	0	0	100	100
1	E	83/89 (93%)	82 (99%)	1 (1%)	0	100	100
1	F	81/89 (91%)	81 (100%)	0	0	100	100
All	All	496/534 (93%)	492 (99%)	4 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2   Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	69/67 (103%)	68 (99%)	1 (1%)	67	29
1	B	67/67 (100%)	66 (98%)	1 (2%)	65	27
1	C	66/67 (98%)	65 (98%)	1 (2%)	65	27
1	D	64/67 (96%)	63 (98%)	1 (2%)	62	24
1	E	67/67 (100%)	65 (97%)	2 (3%)	41	6
1	F	64/67 (96%)	64 (100%)	0	100	100
All	All	397/402 (99%)	391 (98%)	6 (2%)	69	27

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	14	PRO
1	E	4[A]	GLN
1	E	4[B]	GLN
1	B	14	PRO
1	A	14	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	60	HIS
1	E	60	HIS
1	F	47	ASN
1	B	60	HIS
1	C	47	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

24 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	MLY	B	79	1	9,10,11	1.37	1 (11%)	6,11,13	1.44	1 (16%)
1	MLY	A	83	1	9,10,11	0.73	0	6,11,13	1.24	1 (16%)
1	MLY	F	83	1	9,10,11	0.95	0	6,11,13	1.37	1 (16%)
1	MLY	A	79	1	9,10,11	0.77	0	6,11,13	2.09	3 (50%)
1	MLY	F	79	1	9,10,11	1.55	1 (11%)	6,11,13	1.85	2 (33%)
1	MLY	C	25	1	9,10,11	1.05	0	6,11,13	0.92	0
1	MLY	D	34	1	9,10,11	1.43	1 (11%)	6,11,13	1.60	2 (33%)
1	MLY	D	79	1	9,10,11	1.58	1 (11%)	6,11,13	1.28	0
1	MLY	D	83	1	9,10,11	1.34	1 (11%)	6,11,13	0.68	0
1	MLY	C	83	1	9,10,11	1.11	1 (11%)	6,11,13	1.02	1 (16%)
1	MLY	F	25	1	9,10,11	0.81	0	6,11,13	1.40	1 (16%)
1	MLY	A	25	1	9,10,11	1.03	0	6,11,13	1.81	2 (33%)
1	MLY	E	34	1	9,10,11	1.42	1 (11%)	6,11,13	1.46	2 (33%)
1	MLY	E	83	1	9,10,11	0.68	0	6,11,13	1.13	0
1	MLY	E	79	1	9,10,11	1.41	1 (11%)	6,11,13	2.14	3 (50%)
1	MLY	B	83	1	9,10,11	0.95	0	6,11,13	1.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
1	MLY	B	34	1	9,10,11	1.09	1 (11%)	6,11,13	1.48	1 (16%)
1	MLY	C	79	1	9,10,11	1.19	1 (11%)	6,11,13	1.76	2 (33%)
1	MLY	A	34	1	9,10,11	1.93	1 (11%)	6,11,13	1.23	1 (16%)
1	MLY	F	34	1	9,10,11	1.82	1 (11%)	6,11,13	1.57	1 (16%)
1	MLY	E	25	1	9,10,11	1.56	1 (11%)	6,11,13	1.38	1 (16%)
1	MLY	C	34	1	9,10,11	1.07	0	6,11,13	1.53	1 (16%)
1	MLY	B	25	1	9,10,11	1.56	1 (11%)	6,11,13	1.47	2 (33%)
1	MLY	D	25	1	9,10,11	0.84	0	6,11,13	1.16	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	B	79	1	-	4/8/9/11	-
1	MLY	A	83	1	-	0/8/9/11	-
1	MLY	F	83	1	-	2/8/9/11	-
1	MLY	A	79	1	-	6/8/9/11	-
1	MLY	F	79	1	-	2/8/9/11	-
1	MLY	C	25	1	-	0/8/9/11	-
1	MLY	D	34	1	-	0/8/9/11	-
1	MLY	D	79	1	-	4/8/9/11	-
1	MLY	D	83	1	-	2/8/9/11	-
1	MLY	C	83	1	-	0/8/9/11	-
1	MLY	F	25	1	-	4/8/9/11	-
1	MLY	A	25	1	-	1/8/9/11	-
1	MLY	E	34	1	-	2/8/9/11	-
1	MLY	E	83	1	-	0/8/9/11	-
1	MLY	E	79	1	-	1/8/9/11	-
1	MLY	B	83	1	-	0/8/9/11	-
1	MLY	B	34	1	-	5/8/9/11	-
1	MLY	C	79	1	-	2/8/9/11	-
1	MLY	A	34	1	-	4/8/9/11	-
1	MLY	F	34	1	-	3/8/9/11	-
1	MLY	E	25	1	-	5/8/9/11	-
1	MLY	C	34	1	-	0/8/9/11	-
1	MLY	B	25	1	-	3/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	D	25	1	-	4/8/9/11	-

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	34	MLY	CB-CA	5.32	1.60	1.53
1	F	34	MLY	CB-CA	5.05	1.60	1.53
1	D	79	MLY	CB-CA	4.12	1.59	1.53
1	E	34	MLY	CB-CA	3.43	1.58	1.53
1	B	25	MLY	CB-CA	3.30	1.58	1.53

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	79	MLY	CD-CE-NZ	4.02	124.66	113.79
1	F	79	MLY	CD-CE-NZ	3.77	124.00	113.79
1	A	79	MLY	CD-CE-NZ	-3.77	103.58	113.79
1	F	34	MLY	CH2-NZ-CH1	-3.34	101.09	109.73
1	A	25	MLY	CH2-NZ-CH1	-3.01	101.95	109.73

There are no chirality outliers.

5 of 54 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	34	MLY	O-C-CA-CB
1	E	25	MLY	C-CA-CB-CG
1	A	79	MLY	N-CA-CB-CG
1	A	79	MLY	C-CA-CB-CG
1	E	25	MLY	CD-CE-NZ-CH1

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	79	MLY	1	0
1	E	25	MLY	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
2	BDF	A	101	-	12,12,12	0.24	0	18,18,18	0.83	0
2	BDF	F	102	-	12,12,12	0.32	0	18,18,18	0.65	0
2	BDF	C	102	-	12,12,12	0.25	0	18,18,18	0.80	0
2	BDF	F	101	-	12,12,12	0.15	0	18,18,18	0.61	0
2	BDF	C	101	-	12,12,12	0.33	0	18,18,18	1.01	1 (5%)
2	BDF	D	102	-	12,12,12	0.34	0	18,18,18	0.75	0
2	BDF	A	102	-	12,12,12	0.33	0	18,18,18	0.77	0
2	BDF	E	101	-	12,12,12	0.24	0	18,18,18	0.83	0
2	BDF	E	102	-	12,12,12	0.40	0	18,18,18	0.65	0
2	BDF	B	102	-	12,12,12	0.19	0	18,18,18	0.76	0
2	BDF	D	101	-	12,12,12	0.22	0	18,18,18	0.72	0
2	BDF	B	101	-	12,12,12	0.41	0	18,18,18	0.88	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BDF	A	101	-	-	0/3/23/23	0/1/1/1
2	BDF	F	102	-	-	0/3/23/23	0/1/1/1
2	BDF	C	102	-	-	0/3/23/23	0/1/1/1
2	BDF	F	101	-	-	0/3/23/23	0/1/1/1
2	BDF	C	101	-	-	0/3/23/23	0/1/1/1
2	BDF	D	102	-	-	0/3/23/23	0/1/1/1
2	BDF	A	102	-	-	0/3/23/23	0/1/1/1
2	BDF	E	101	-	-	0/3/23/23	0/1/1/1
2	BDF	E	102	-	-	0/3/23/23	0/1/1/1
2	BDF	B	102	-	-	0/3/23/23	0/1/1/1
2	BDF	D	101	-	-	0/3/23/23	0/1/1/1
2	BDF	B	101	-	-	0/3/23/23	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	101	BDF	O4-C4-C5	2.03	113.89	109.99

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	85/89 (95%)	0.87	3 (3%)	44	43	6, 10, 17, 81	0
1	B	85/89 (95%)	0.86	3 (3%)	44	43	6, 10, 19, 83	0
1	C	85/89 (95%)	1.09	6 (7%)	16	16	6, 10, 19, 84	0
1	D	83/89 (93%)	0.62	2 (2%)	59	57	7, 10, 16, 28	0
1	E	84/89 (94%)	0.80	4 (4%)	30	30	6, 9, 16, 69	0
1	F	83/89 (93%)	0.55	0	100	100	6, 10, 16, 36	0
All	All	505/534 (94%)	0.80	18 (3%)	42	42	6, 10, 19, 84	0

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	89	THR	18.2
1	B	90	ASN	16.0
1	C	90	ASN	13.4
1	A	90	ASN	13.2
1	B	89	THR	12.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	MLY	D	34	11/12	0.74	0.23	19,28,33,34	0
1	MLY	C	34	11/12	0.81	0.22	15,18,29,30	0
1	MLY	B	79	11/12	0.81	0.28	17,25,39,39	0
1	MLY	F	34	11/12	0.82	0.21	16,24,32,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	MLY	A	34	11/12	0.82	0.35	15,21,38,38	0
1	MLY	F	79	11/12	0.86	0.28	10,19,35,36	0
1	MLY	C	79	11/12	0.87	0.21	9,17,29,30	0
1	MLY	D	79	11/12	0.87	0.25	8,15,34,34	0
1	MLY	A	79	11/12	0.87	0.26	13,24,39,39	0
1	MLY	E	79	11/12	0.89	0.21	8,14,33,33	0
1	MLY	E	25	11/12	0.89	0.23	9,13,32,33	0
1	MLY	B	25	11/12	0.91	0.22	10,14,35,35	0
1	MLY	F	83	11/12	0.91	0.15	10,13,29,30	0
1	MLY	D	25	11/12	0.91	0.19	12,15,33,33	0
1	MLY	E	34	11/12	0.91	0.21	9,16,35,35	0
1	MLY	B	34	11/12	0.92	0.15	13,20,29,29	0
1	MLY	F	25	11/12	0.93	0.22	10,13,32,33	0
1	MLY	A	25	11/12	0.94	0.16	10,14,32,32	0
1	MLY	C	25	11/12	0.94	0.12	10,14,18,19	0
1	MLY	D	83	11/12	0.95	0.11	7,9,14,15	0
1	MLY	A	83	11/12	0.95	0.12	8,9,18,21	0
1	MLY	C	83	11/12	0.96	0.09	6,9,15,17	0
1	MLY	B	83	11/12	0.96	0.09	9,10,13,16	0
1	MLY	E	83	11/12	0.96	0.10	7,8,15,16	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BDF	F	101	12/12	0.71	0.21	13,26,27,27	0
2	BDF	D	101	12/12	0.83	0.17	15,17,18,19	0
2	BDF	C	101	12/12	0.92	0.14	7,7,9,10	24
2	BDF	A	101	12/12	0.92	0.14	6,7,8,9	24
2	BDF	B	102	12/12	0.92	0.16	8,11,14,15	24
2	BDF	F	102	12/12	0.94	0.15	7,8,9,9	24
2	BDF	D	102	12/12	0.95	0.14	6,6,7,8	24
2	BDF	B	101	12/12	0.96	0.10	9,9,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\mathrm{\AA}^2$)	Q<0.9
2	BDF	E	102	12/12	0.96	0.15	5,6,6,8	24
2	BDF	C	102	12/12	0.96	0.16	6,8,8,9	24
2	BDF	A	102	12/12	0.96	0.10	7,9,12,13	0
2	BDF	E	101	12/12	0.97	0.14	5,6,6,7	24

6.5 Other polymers ⓘ

There are no such residues in this entry.